

Appendix B – T-REX Model Description

5. Introduction

This spreadsheet based model calculates the decay of a chemical applied to foliar surfaces for single or multiple applications. It uses the same principle as the batch code models FATE and TERREEC for calculating terrestrial estimates exposure (TEEC) concentrations on plant surfaces following application. A first order decay assumption is used to determine the concentration at each day after initial application based on the concentration resulting from the initial and additional applications. The decay is calculated by from the first order rate equation:

$$C_T = C_i e^{-kT}$$

or in log form:

$$\ln (C_T/C_i) = -kT$$

Where:

C_T = concentration at time T = day zero.

C_i = concentration, in parts per million (PPM) present initially (on day zero) on the surfaces. C_i is calculated based on Kenaga and Fletcher by multiplying the C_i based on the Kenaga nomogram (Hoerger and Kenaga, (1972) as modified Fletcher (1994). For maximum concentration the application rate, in pounds active ingredient per acre, is multiplied by 240 for Short Grass, 110 for Tall Grass, and 135 for Broad leafed plants/small insects and 15 for fruits/pods/lg insects. Additional applications are converted from pounds active ingredient per acre to PPM on the plant surface and the additional mass added to the mass of the chemical still present on the surfaces on the day of application.

K = If the foliar dissipation data submitted to EFED are found scientifically valid and statistically robust for a specific pesticide, the 90% upper confidence limit of the mean half-lives should be used. When scientifically valid, statistically robust data are not available TETT recommends the using a default half-life value of 35 days. The use of the 35 day half-life is based on the highest reported value (36.9 days) reported by Willis and McDowell (Pesticide persistence on foliage, Environ. Contam.Toxicol, 100:23-73, 1987).

T = time, in days, since the start of the simulation. The initial application is on day 0. The simulation is designed to run for 365 days.

The program calculates concentration on each type of surface on a daily interval for one year. The maximum concentration during the year are calculated for both maximum and mean residues. The inputs used to calculate the amount of the chemical present are in highlighted in light blue on the spread sheet. Outputs are in yellow. The inputs required are:

Application Rate:

The maximum label application rate (in pounds ai/acre)

Half-life: The degradation half-life for the dominate process(in days)

Frequency of Application: The interval between repeated applications, from the label (in days)

Maximum # Applications per year:From the label

5. Avian Species

For calculating dose-based RQs in birds, the upper bound and mean Kenaga residue values are adjusted for avian class and food consumption based on the following scaling factor (USEPA, 1993):

$$FI (g/d) = 0.648 (g \text{ bw})^{0.651}$$

For the 3 avian weight classes considered (20, 100 and 1000 g), this results in % body weight consumption of:

Weight(g)	FI	wet FI	% bw consumed
20	4.555599463	22.77799731	114
100	12.98897874	64.94489369	65
1000	58.15338588	290.7669294	29

5. Dose-Based Acute RQs

Dose-based acute RQs are then calculated using the formula:

$$RQ = \text{adjusted EEC} / LD_{50} \text{ or NOAEL}$$

where the adjusted EEC is considered to be the daily dose weighted for % body weight consumed of a given food source.

5. Dietary-Based RQs

For dietary-based RQs, two values are given for each food group. First, the consumption-weighted RQ for each weight class (20, 100, and 1000g birds) is displayed and calculated using the equation:

$$RQ = EEC / ((LC_{50} \text{ or NOAEC}) / (\%bw \text{ consumed}))$$

In the second method, no adjustment is made for consumption differences among the weight classes. This RQ is calculated:

$$RQ = EEC/LC_{50} \text{ or NOAEC}$$

3. Mammalian Species

A. Dose-Based RQs

For calculating dose-based RQs in mammals, the upper bound and mean Kenaga values are adjusted for mammalian class and food consumption (0.95, 0.66 and 0.15 body weight for herbivores and insectivores and 0.21, 0.15, and 0.03 body wt. for granivores). Dose-based acute and chronic RQs are then calculated by dividing the adjusted EECs (daily dose) by the LD₅₀ or NOAEL.

5. Dietary-Based RQs

Dietary-based RQs are calculated using the equation:

$$RQ = EEC/((LC_{50} \text{ or NOAEC})/(\% \text{ bw consumed}))$$

4. New Version Notes

A new look is used in this update in an effort to decrease confusion and increase transparency in the risk assessment process. This version of T-REX (v1.1) incorporates the ability to calculate EECs and RQs for upper bound and mean residues. Mean residues are calculated exactly as the upper bound residues are, except the corresponding Kenaga values are: 85 for Short Grass, 36 for Tall Grass, and 45 for Broad leafed plants/small insects and 7 for fruits/pods/lg insects.

5. References

- Fletcher, J.S., J.E. Nellessen and T. G. Pfleeger. 1994. Literature review and evaluation of the EPA food-chain (Kenaga) nomogram, an instrument for estimating pesticide residues on plants. *Environ. Tox. And Chem.* 13(9):1383-1391.
- Hoerger, F. and E.E. Kenaga. 1972. Pesticide residues on plants: correlation of representative data as a basis for estimation of their magnitude in the environment. IN: F. Coulston and F. Corte, eds., *Environmental Quality and Safety: Chemistry, Toxicology and Technology*. Vol 1. Georg Theime Publishers, Stuttgart, Germany. Pp. 9-28.
- USEPA. 1993. *Wildlife Exposure Factors Handbook*. Volume I of II. EPA/600/R-93/187a. Office of Research and Development, Washington, D. C. 20460.
- Willis and McDowell. 1987. Pesticide persistence on foliage. *Environ. Contam. Toxicol.* 100:23-73.